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# A novel internal combustion engine utilizing internal hydrogen production for improved efficiency – A theoretical concept

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## ARTICLE INFO

### Article history:

Received 1 April 2014

Received in revised form

13 September 2014

Accepted 15 September 2014

Available online 8 October 2014

### Keywords:

Thermodynamic cycle

Internal combustion engines

Diesel engines

Internal hydrogen production

Steam reforming

## ABSTRACT

Starting from the baseline of a Diesel engine, we show that with a suitable in-cylinder catalyst and well controlled injection of fuel and steam mixture during a certain period in the compression stage, a significant increase in the ideal cycle efficiency is achievable (from 67% to 78% for an initial compression ratio of 25). In such an arrangement, the fuel injection session comprises a two-stage process. In the first stage, fuel and water are injected into the hot previously compressed cylinder charge over the catalyst. Residual heat is absorbed due to a steam reforming process to produce hydrogen. The heat absorption cools the compressed mixture and enables a higher compression ratio up to the maximum allowed pressure, while the temperature of the cylinder charge remains constant. In the second stage, only fuel is injected to initiate combustion while the absorbed heat (of the first stage) is released through the hydrogen oxidation. Essentially, the absorbed heat is exploited to produce extra hydrogen fuel, which increases the cycle efficiency.

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## Introduction

The cycle starts at point 1 (Fig. 1) where the piston is at BC (Bottom Centre) and the trapped charge (air for DI engines) is at STP conditions. The basic Diesel cycle is shown by points 1–2–3–4–1. In the present new cycle, the charge is compressed by the up-moving piston from state 1 to 2b. During compression, at point 2a, a well prepared mixture of fuel and steam is introduced to the cylinder in the presence of a suitable catalytic surface. In the first stage, when injection takes place, residual heat is absorbed due to a steam reforming

process to produce hydrogen. The heat absorption cools the compressed mixture and enables a higher compression ratio up to the maximum allowed pressure, while the temperature of the cylinder charge is kept constant (2a–2b). In the second stage, after injection has ended (2b), the absorbed heat (of the first stage) is being used during the combustion stage, when the hydrogen undergoes combustion. Essentially, the absorbed heat is exploited to produce extra hydrogen fuel, which increases the cycle efficiency. That contribution is unique to the combined steam and fuel injection in the present study. The fuel injection rate has to be controlled such that the combustion process (of the injected fuel and the previously

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<http://dx.doi.org/10.1016/j.ijhydene.2014.09.079>

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## Nomenclature

|          |                                      |
|----------|--------------------------------------|
| $c_p$    | heat capacity at constant pressure   |
| $c_v$    | heat capacity at constant volume     |
| $m$      | mass                                 |
| $P$      | pressure                             |
| $Q$      | heat                                 |
| $R$      | gas constant                         |
| $T$      | temperature                          |
| $t$      | time                                 |
| $V$      | volume                               |
| $K_{p1}$ | equilibrium constant (eq. (1))       |
| $K_{p2}$ | equilibrium constant (eq. (2))       |
| $W$      | work                                 |
| $x$      | CO <sub>2</sub> production (Table 1) |
| $y$      | methane conversion (Table 1)         |
| $\eta$   | efficiency                           |

## Indices

|   |               |
|---|---------------|
| 0 | ambient (STP) |
|---|---------------|

generated hydrogen) is performed from 2b to 3 under constant pressure conditions. Combustion thus takes place between 2b and 3, while injecting the rest of the fuel.

The overall amount of combusting fuel would be the injected fuel of 2a→2b and 2b→3, less the fuel consumed during 2a→2b (by the hydrogen generating reactions), plus the hydrogen fuel generated during 2a→2b. In total, that should have a higher calorific value than just the amount of supplied fuel (during 2a→3 combined), as the hydrogen generating reactions are endothermic in total. If the same amount of supplied fuel is used in a standard Diesel cycle of the same maximum pressure, the fuel injection will take place between 2 and 3. We note however that in the modified-Diesel cycle described here, hydrogen combustion takes place past point 2b, as it actually carries energy of the prior injected fuel (during 2a→2b). Nevertheless, the overall indicatoric work (area of  $P$ – $V$  diagram) is larger for the same total amount of injected fuel as in a standard comparable Diesel cycle, hence its superior efficiency to the latter. The point 2a is chosen as the minimal temperature which would still suffice for a significant amount of water steam reformation. On the other hand, the lower that temperature is, the more heat could be absorbed from the compression stroke, hence an optimization of that point could be achieved. Another factor to consider is the rate of catalyzed reaction, which increases with temperature. Using modern catalysts [1,2] can enable a high enough rate, namely, of a time shorter than the time of the compression stroke, at a workable temperature. For this task, a metal-based catalyst with a suitable effective surface area could fit (e.g. Ni/MgAl<sub>2</sub>O<sub>4</sub> or Ni/ZrO<sub>2</sub>). Larger Diesel engines, however, of slower rpm's could accommodate a wider selection of catalysts, or lower compression temperatures. Process 3–4 is an isentropic expansion, and 4–1 designates the gas exchange process.

In order to evaluate the new cycle efficiency, we use the following approach.

## Thermo-chemistry of steam reforming

To model the steam reforming process, we use a simplified system of Methane–Water, and consider chemical equilibrium reactions between them. We assume the dominant simultaneous reactions to be:

1.  $\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2$
2.  $\text{CH}_4 + \text{H}_2\text{O} \rightleftharpoons \text{CO} + 3\text{H}_2$

With the purpose of reducing times required for equilibriums, the reactions occur in the presence of a catalyst. The first reaction is moderately endothermic, while the second is highly endothermic. The Equilibrium constants [3] for these two reactions are presented in Fig. 2.

The importance of temperature to these reactions could be realized from Fig. 2. An increase in the temperature from 900 K to 1200 K, for example, results in an increase of 3 orders of magnitude in the equilibrium constant in favour of H<sub>2</sub> production.

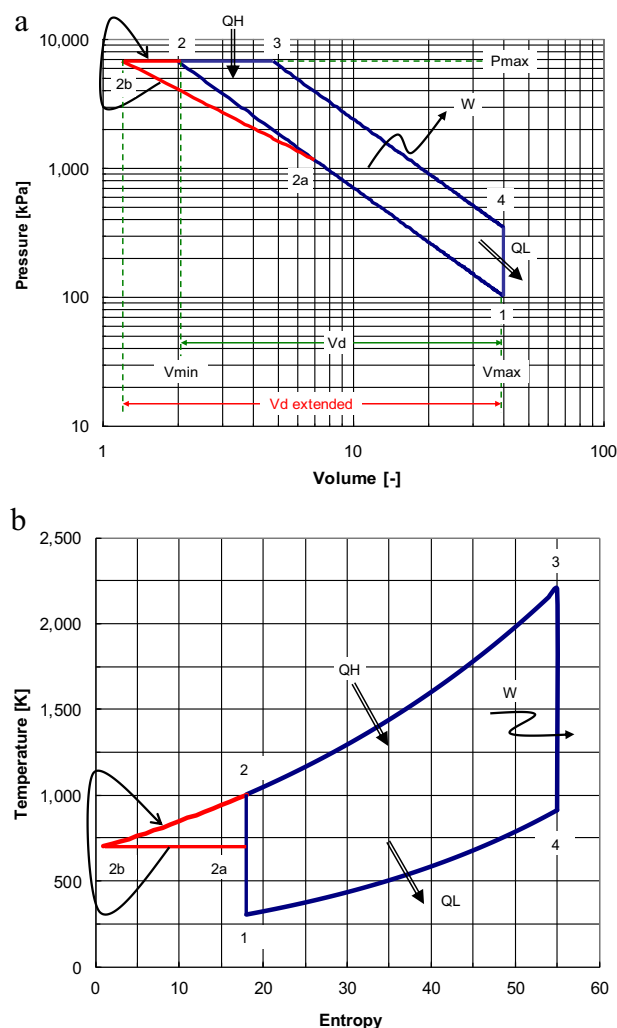


Fig. 1 – The thermodynamic cycles of Diesel and modified-Diesel on a: a)  $P$ – $V$  diagram b)  $T$ – $s$  diagram.

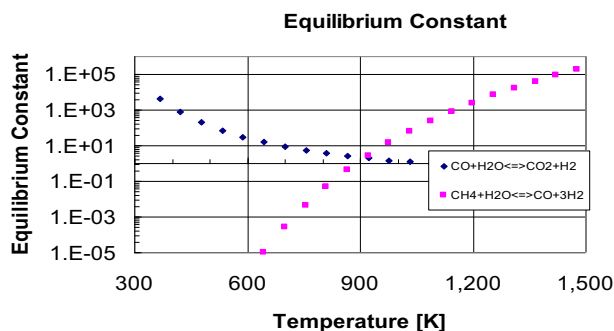


Fig. 2 – Equilibrium constants for reaction 1 and 2 at different temperatures.

We calculate the  $H_2$  production vs. temperature and pressure in terms of mole fraction (0 = no conversion, 1 = full conversion), with according to Table 1: here  $x$  denotes  $CO_2$  production,  $y$  denotes Methane conversion and  $x + 3y$  denotes  $H_2$  production per one mole  $CH_4$ . Equilibrium relations, for the two respective reactions, are:

$$K_{p1} = \frac{\left(\frac{x}{2+2y}\right)\left(\frac{x+3y}{2+2y}\right)}{\left(\frac{-x+y}{2+2y}\right)\left(\frac{1-x-y}{2+2y}\right)} \left(\frac{P}{P_0}\right)^0 \quad (1)$$

$$K_{p2} = \frac{\left(\frac{-x+y}{2+2y}\right)\left(\frac{x+3y}{2+2y}\right)^3}{\left(\frac{1-y}{2+2y}\right)\left(\frac{1-x-y}{2+2y}\right)} \left(\frac{P}{P_0}\right)^2 \quad (2)$$

Starting from a mixture of Methane and steam at a mole ratio of 1:1, results are plotted in Fig. 3. We observe that full conversion may practically occur at around 1200 K at a pressure of 1 atm, and it may occur at 900 K at a pressure of 60 atm. We also note that the ignition temperatures of  $H_2$  and  $CH_4$  at 1 atm are 773 K and 853 K respectively, while it may decrease at higher pressures. In practical terms, during compression, the charge temperature is kept low (below the ignition temperature) owing to the internal endothermic steam reforming reactions. For example, when we consider a low temperature of 700 K at state no. 2a, the conversion efficiency of the steam reforming process is much lower than 100%, but the unconverted fuel however will burn during the combustion process in the subsequent stage.

### Engine cycle thermodynamics

Considering a classic Diesel engine cycle, the four basic stages are: 1–2: isentropic compression, 2–3 constant-pressure combustion, 3–4 isentropic expansion, and 4–1 scavenging (thermodynamically equivalent to constant-volume cooling). Numbers correspond to state-points in Fig. 1. Generally, efficiency would be higher for a higher compression ratio. However, maximum pressure in the cycle is limited by practical structural considerations of the engine.

Table 1 – Mole fractions for reactions 1 and 2.

|        | Initial | End         |
|--------|---------|-------------|
| CO     | 0       | $-x + y$    |
| $H_2O$ | 1       | $1 - x - y$ |
| $CO_2$ | 0       | $x$         |
| $H_2$  | 0       | $x + 3y$    |
| $CH_4$ | 1       | $1 - y$     |
| Total  | 2       | $2 + 2y$    |

In this study, an alteration of this classic Diesel cycle is suggested as to enhance thermodynamic efficiency (by waste heat re-use), by making use of steam reforming. At some point after compression has started, (2a), injection of the methane (and if needed injection of more water or steam) into the cylinder is started, while compression is still ongoing. This steam mixture, hitting an appropriate catalyst installed in the cylinder reacts endothermally (absorbing heat). As such, the in-cylinder temperature could be controlled during the ongoing compression (2a–2b) by controlling the rate of fuel-steam mixture injection. For maximum heat absorption it is best to maintain a constant temperature by steam injection. Once compression ends (2b), combustion starts, where the previously formed Hydrogen combusts with main injected fuel (injected during combustion, as in classic Diesel engine).

We evaluate the efficiency of this cycle by considering the work and heat energies in every stage.

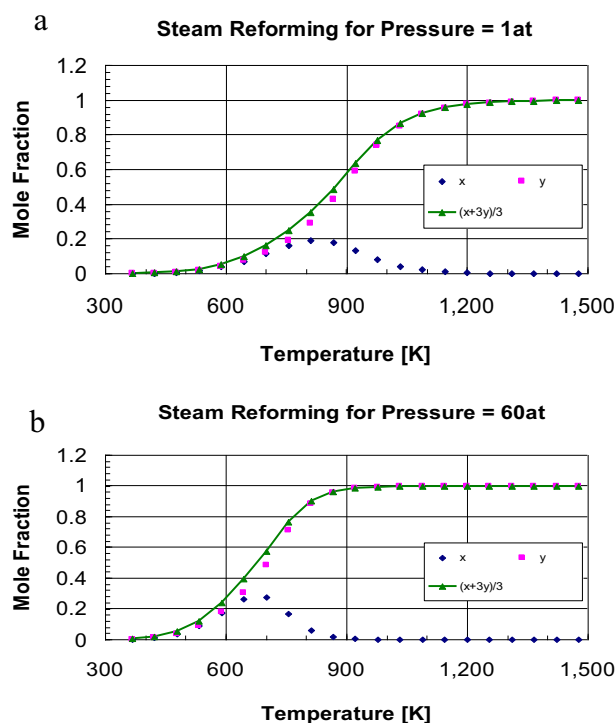


Fig. 3 – Mole fractions at different temperatures at: a) 1 atm. b) 60 atm.

Isentropic compression (1–2a):

$${}_1W_{2a} = mc_v(T_{2a} - T_1) \quad {}_1Q_{2a} = 0 \quad (3)$$

Isothermic compression (2a–2b):

$${}_2aW_{2b} = mRT_{2a,2b} \ln\left(\frac{V_{2b}}{V_{2a}}\right)$$

$${}_2aQ_{2b} = {}_2aW_{2b} \quad (\text{the heat that is absorbed by steam reforming}) \quad (4)$$

Isobaric combustion (2b–3):

$${}_2bW_3 = P_{2b,3}(V_3 - V_{2b}) \quad {}_2bQ_3 = mc_p(T_3 - T_{2b}) \quad (5)$$

Isentropic expansion (3–4):

$${}_3W_4 = mc_v(T_1 - T_4) \quad {}_3Q_4 = 0 \quad (6)$$

Scavenging (4–1):

$${}_4W_1 = 0 \quad {}_4Q_1 = mc_v(T_1 - T_4) \quad (7)$$

The efficiency is then evaluated as the net work over heat input:

$$\eta = \frac{{}_1W_{2a} + {}_2aW_{2b} + {}_2bW_3 + {}_3W_4 + {}_4W_1}{{}_2aQ_{2b} + {}_2bQ_3} \quad (8)$$

(we note that  ${}_2aQ_{2b}$  is negative).

A comparable standard Diesel cycle (of the same maximum pressure and volume) would have the efficiency:

$$\eta = \frac{{}_2W_3 + {}_3W_4 + {}_4W_1}{{}_2Q_3} \quad (9)$$

Fig. 4 shows the effect of the internal steam reforming process on the thermodynamic efficiency of a standard Diesel cycle for different compression ratio's and engine loads, for ambient STP conditions and catalytic temperature of 700 K.

The engine load is represented by the cut-off ratio, i.e., by  $V_3/V_2$ , the volume ratio (=the temperature ratio) over the combustion process. We note that the improvement of the cycle efficiency increases for higher compression ratio's. Under these conditions, the portion of the piston stroke that remains after achieving 700 K is longer and thus more energy is recovered by the endothermic reactions. We also note that the improvement increases as the engine load decreases; under these conditions, the amount of fuel that is added during the combustion process is lower and thus the portion of the energy recovering as related to the total energy is more significant.

Fig. 4 suggests that for a compression ratio of 1:25 and cut-off ratio of 1.8, we obtain theoretical cycle efficiency improvement from 67% to 78%. The improved efficiency can be visualized in Fig. 1a and b as the added area of the graphed cycle, which represents an added indicatonic work.

## Conclusions

The steam and fuel mixture have to be injected during the compression stroke when the temperature exceeds 700 K, for the chemical reactions of steam reformation to produce a realistically significant amount of hydrogen (above 80% steam conversion ratio, using a catalyst. See Fig. 2). Then the compression stroke continues until the maximum allowed pressure is reached. This is followed by the isobaric combustion process while the hydrogen replaces some of the fuel. In an engine of initial 1:25 compression ratio (90 atm. maximum pressure), efficiency could be theoretically improved from 66% to 75%, by an appropriate steam reforming.

Achieving a higher efficiency without elevating the maximum temperature produces, in effect, a reduction in pollution per generated power. In addition, because hydrogen combustion is involved, it is expected that the amount of CO and HC emission levels will be very low as compares to those

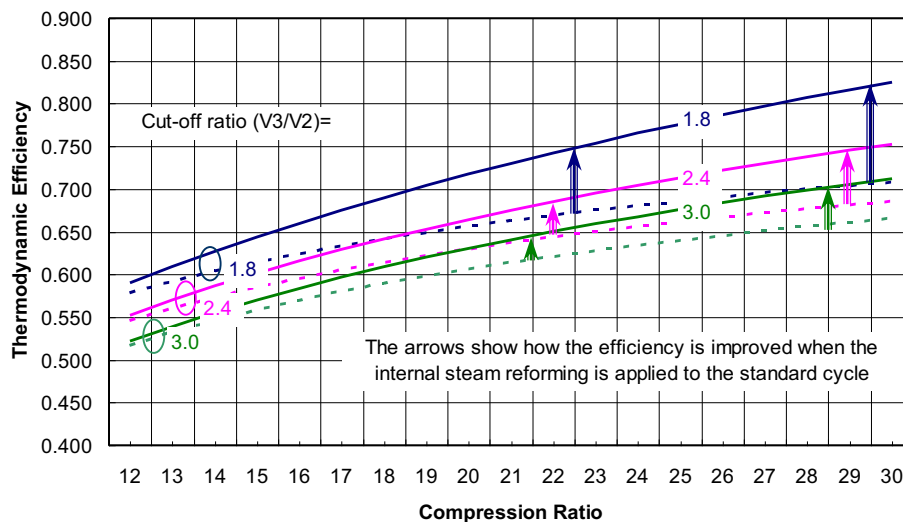


Fig. 4 – The effect of the internal steam reforming on the thermodynamic efficiency of a standard cycle vs. compression ratio and engine load (cut-off ratio).

emitted from conventional Diesel engine. It is also important to note that since the temperature of the cylinder charge at the end of the compression stroke is much lower than that of the conventional Diesel engine, and since the  $\text{NO}_x$  production depends exponentially on the flame temperature (the flame temperature depends also on the charge temperature which is lower in the present case), the  $\text{NO}_x$  emission level is also expected to be lower.

Results depend on maximum allowed pressure in the cylinder (the higher the better), which also affect the steam reforming conversion ratio (hydrogen production).

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